Semi-definite Relaxation of Quadratic Assignment Problems based on Nonredundant Matrix Splitting

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Abstract

Quadratic Assignment Problems (QAPs) are known to be among the most challenging discrete optimization problems. Recently, a new class of semi-definite relaxation models for QAPs based on matrix splitting has been proposed [17, 20]. In this paper, we consider the issue of how to choose an appropriate matrix splitting scheme so that the resulting relaxation model can provide a strong bound. For this, we introduce a new notion of the so-called redundant and non-redundant matrix splitting. We show that the relaxation based on a non-redundant matrix splitting can provide a stronger bound than a redundant one. We then propose to follow the minimal trace principle to find such a non-redundant matrix splitting. Based on the minimal trace principle, three matrix splitting schemes are derived and coincidentally, two of them had already been used in [17, 20]. A new matrix splitting, called sum-matrix splitting, is introduced. A similar procedure as in [20] is used to construct the SDP relaxation model. Numerical experiments show the bound based on the sum-matrix splitting is very competitive with existing bounds including the bounds based on other matrix splitting schemes.

Key words. Quadratic Assignment Problem (QAP), Semidefinite Programming (SDP), Matrix Splitting, Relaxation, Lower Bound.

1 Introduction

Given matrices A, B, we consider the quadratic assignment problem (denoted by QAP) of the following form

$$\min_{X\in\Pi} \operatorname{Tr}\big(AXBX^T\big) \tag{1}$$

where $\operatorname{Tr}(\cdot)$ denotes the trace of a matrix and Π is the set of permutation matrices. We assume that A and B are $n \times n$ symmetric matrices throughout this paper. QAP was first introduced by Koopmans and Beckmann [15] for facility location and has applications

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in many areas such as chip design [7, 12], image analysis and processing [18, 24], and communications [1]. For more applications of QAP, we refer to the survey paper [16].

It is well-known that QAP is NP-hard. Searching for the global solution of QAP usually involves the branch and bound (B&B) method. Crucial issue in the B&B method is how to compute strong lower bounds efficiently. A lot of papers have been devoted to deriving strong yet cheap relaxation models for QAP, we refer the readers to [3, 5, 16] for reviews of these bounds and an up-to-date website QAPLIB[1] for the practical performance of them on collections of QAP instances [4].

Among all the relaxation models, we are particularly interested in the semidefinite relaxation models which can provide relatively stronger lower bounds compared with other relaxations based on linear and quadratic programming. A popular way to derive the SDP relaxations of QAP is to relax the rank-1 matrix $vec(X)vec(X)^T$ to a $n^2 \times n^2$ positive semidefinite with additional constraints on the matrix elements, where $vec(X)$ denotes the lifted n^2 vector obtained from X by stacking its columns sequently into a long vector. Though many efforts have been made to reduce the computational cost of solving the SDP relaxation based on the gram matrix $vec(X)vec(X)^T$ [21, 2, 8], the large number $O(n^4)$ of variables and constraints in these relaxations still make them formidable for medium size QAP instances with the current computation facilities. Recently, Ding and Wolkowicz [9] introduced a new SDP relaxation of QAP based on matrix lifting. The resulting SDP model has only $O(n^2)$ of variables and constraints and thus can be solved using open source SDP solvers for QAPs of size $n \leq 30$, though it still remains a computational challenge for $n \geq 30$.

In our recent work [20], a new framework to derive cheap and strong SDP relaxation for QAP based on various matrix splitting schemes was introduced. It is shown that some relaxation models in [17, 20] can provide competitive bounds comparing with other relaxation models in the literature. However, since there is a large variety in matrix splitting schemes, it is unclear which splitting scheme can lead to the strongest relaxation.

In this paper, we are mainly concerned with the issue of how to choose a matrix splitting scheme so that the resulting relaxation model can provide a strong bound. For this, we first introduce a new notion of the so-called redundant and non-redundant matrix splitting. We show that for any given redundant matrix splitting, there exists a corresponding non-redundant matrix splitting such that the resulting SDP relaxation can provide a stronger bound. To find such a non-redundant matrix splitting, we propose to solve some auxiliary SDP problems following the minimal trace principle. Based on the minimal trace matrix splitting, three matrix splitting schemes are derived and their relationships with existing matrix splitting schemes are discussed. Two of them are precisely the matrix splitting schemes used in [17, 20]. A new matrix splitting, called sum-matrix splitting, is introduced and we employ a similar procedure as in [20] to derive the SDP relaxation model.

To further help select a good splitting scheme, we investigate the theoretical properties of the optimal solutions to these auxiliary SDP problems and use these characterizations to study the relationships between different splitting schemes and their associated SDP relaxations. Based on the rank information at the optimal solution to the auxiliary problem, we present a new implementation of the relaxation model which leads to substantial improvement over the implementation in [20]. Numerical experiments show the bound based on the new splitting schemes and implementation is very competitive with existing bounds including the bounds based on other matrix splitting schemes, and can be computed more

[1] http://www.seas.upenn.edu/qaplib/

effectively.

The paper is organized as follows. In Section 2, we present a minimal trace PSD matrix splitting scheme. We first show that compared with the SDP relaxation associated with a redundant matrix splitting, the SDP relaxation for QAPs based on a non-redundant PSD splitting can provide a strong lower bound. In particular, we show that the minimal trace PSD matrix splitting is non-redundant and is identical to the orthogonal PSD matrix splitting. In Section 3, we discuss the minimal trace one-matrix splitting scheme and minimal trace sum-matrix splitting scheme. We give conditions under which these two splitting schemes are non-redundant and the SDP relaxations based on these two splitting schemes can also provide strong lower bounds. In Section 4, we present the SDP relaxation models of QAPs based on the three matrix splitting schemes. Numerical experiments on selected QAP instances from QAPLIB [4] are presented in Section 5.

A few sentences about the notation. Throughout this paper, we use upper case letters to denote matrices and lower case letters for vectors. $E \in \Re^{n\times n}$ denotes the matrix whose elements equal one and $e \in \Re^n$ denotes the vector whose elements equal one. $\mathcal{S}^n$ denotes the set of $n \times n$ real symmetric matrices and $\mathcal{S}^n_+$ denotes the set of $n \times n$ symmetric positive semi-definite (PSD) matrices. We use $X \succeq 0$ to denote $X \in \mathcal{S}^n_+$ and $X \geq 0$ to denote $X_{ij} \geq 0$ for all i, j. $[X]_{ij}$ denotes ith row jth column element of matrix X. For a given symmetric matrix B, $\operatorname{diag}(B)$ denotes the vector consisting of the diagonal elements of B. For a vector d, $\operatorname{diag}(d)$ denotes the diagonal matrix whose diagonal is d. Let $\max(B)$ (or $\min(B)$) denote the column vector whose i-th component is the maximal element (or minimal element) in the i-th row (denoted by $B_{i,:}$) of B. $\mathcal{L}_2(B)$ denotes the column vector whose i-th component is the 2-norm of i-th row of matrix B. $\lambda_{\max}(B)$ and $\lambda_{\min}(B)$ denote the largest eigenvalue and the smallest eigenvalue, respectively.

2 Redundant and Non-redundant Matrix Splitting

As shown in [20], there exist various matrix splitting schemes for a given matrix B and it is unclear that which splitting can lead to the strongest relaxation. In this section, we first introduce a new notion of the so-called redundant and non-redundant matrix splitting and show that for any given redundant matrix splitting, there exists another non-redundant matrix splitting that can provide a stronger relaxation. To find such a non-redundant PSD splitting, we refer to the minimal trace principle. The relationship between the non-redundant matrix splitting based on minimal trace principle and the orthogonal PSD splitting schemes considered in [20] will be discussed as well.

We start with the following definition from [20].

Definition 2.1. *Given matrix B, we call matrix pair (B_1, B_2) a positive semidefinite (PSD) matrix splitting of B if it satisfies*

$$B = B_1 - B_2, \; B_1, B_2 \succeq 0.$$

As pointed out in [20], there exist many PSD matrix splitting schemes. If a PSD splitting (B_1, B_2) of matrix B is available, then we can obtain the following SDP relaxation for QAPs

$$\mu_1(B_1, B_2) = \min_{Y \in \bar{\Upsilon}_1(B_1,B_2)} \operatorname{Tr}(AY), \tag{2}$$

where the feasible set $\bar{\mathrm{Y}}_1(B_1, B_2)$ is defined by

$$\bar{\mathrm{Y}}_1(B_1, B_2) = \left\{ \begin{array}{c|c} Y \in \mathcal{S}^n, & Y = Y_1 - Y_2, \\ X \in \Re^{n\times n} & Y_1 - XB_1X^T \succeq 0, \quad Y_2 - XB_2X^T \succeq 0, \\ & \mathrm{diag}\,(Y_1) = X\mathrm{diag}\,(B_1), \quad Y_1e = XB_1e, \\ & \mathrm{diag}\,(Y_2) = X\mathrm{diag}\,(B_2), \quad Y_2e = XB_2e, \\ & Xe = X^Te = e, \quad X \geq 0 \end{array} \right\}. \tag{3}$$

We now introduce the following definition.

Definition 2.2. *A PSD matrix splitting (B_1, B_2) is said to be redundant (or non-redundant) if there exists (or does not exist) a nonzero matrix $R \succeq 0$ satisfying*

$$B_1 - R \succeq 0, \quad B_2 - R \succeq 0.$$

From the above definition, we immediately have

Proposition 2.3. *Given a matrix B. A PSD matrix splitting (B_1, B_2) is non-redundant if and only if 0 is the optimal solution of the following SDP*

$$\max \quad \mathrm{Tr}(R) \tag{4}$$

$$s.t. \quad B_1 - R \succeq 0, B_2 - R \succeq 0, R \succeq 0. \tag{5}$$

We next recall a well-known result regarding the doubly stochastic matrices. A real $n \times n$ matrix $M = (M_{ij})$ is doubly stochastic if the entries of M are non-negative, and each row and column of M sums to 1 [19]. The following result is from [19](Theorem 2, Birkhoff's theorem).

Lemma 2.4. *The set of $n \times n$ doubly stochastic matrices is a convex set whose extreme points are the permutation matrices.*

Based on Lemma 2.4, we first establish a result regarding a redundant PSD splitting.

Theorem 2.5. *If a PSD matrix splitting (B_1, B_2) of the matrix B is redundant with matrix R, then we have*

$$\bar{\mathrm{Y}}_1(B_1 - R, B_2 - R) \subseteq \bar{\mathrm{Y}}_1(B_1, B_2), \tag{6}$$

where $\bar{\mathrm{Y}}_1(\cdot)$ is the set as defined in (3).

Proof. Since the PSD matrix splitting (B_1, B_2) is redundant, there exists nontrivial $R \succeq 0 \in \mathcal{S}^n$ such that

$$B_1 - R \succeq 0, \quad B_2 - R \succeq 0.$$

Clearly, $(B_1 - R, B_2 - R)$ is also a PSD splitting of B.

Now let $Y \in \bar{\mathrm{Y}}_1(B_1 - R, B_2 - R)$. From (3), there exist $Y_1,\ Y_2 \in \mathcal{S}^n$ and $X \in \Re^{n\times n}$ such that

$$Y = Y_1 - Y_2, \tag{7}$$

$$Y_1 - X(B_1 - R)X^T \succeq 0, \quad Y_2 - X(B_2 - R)X^T \succeq 0, \tag{8}$$

$$\mathrm{diag}\,(Y_1) = X\mathrm{diag}\,(B_1 - R), \quad Y_1e = X(B_1 - R)e, \tag{9}$$

$$\mathrm{diag}\,(Y_2) = X\mathrm{diag}\,(B_2 - R), \quad Y_2e = X(B_2 - R)e, \tag{10}$$

$$Xe = X^Te = e, \quad X \geq 0. \tag{11}$$

Note from (11) that X is a $n \times n$ doubly stochastic matrix. By Lemma 2.4, X can be expressed as a convex combination of permutation matrices. However, Caratheodory's theorem [22] guarantees that a point in an m-dimensional compact convex set may be expressed as a convex combination of at most $m+1$ extremal points of that set. The $n \times n$ doubly stochastic matrices form a $n^2 - 2n + 1$-dimensional set, so an arbitrary doubly stochastic matrix may be expressed as a convex combination of at most $n^2 - 2n + 2$ permutation matrices. Let $\hat{n} = n^2 - 2n + 2$. Then there exist $\hat{X}_i \in \Pi$ and $\lambda_i \in \Re_+$, $i = 1, \ldots, \hat{n}$, with $\sum_{i=1}^{\hat{n}} \lambda_i = 1$, such that

$$X = \sum_{i=1}^{\hat{n}} \lambda_i \hat{X}_i, \tag{12}$$

Define

$$Y_R = \sum_{i=1}^{\hat{n}} \lambda_i \hat{X}_i R \hat{X}_i^T. \tag{13}$$

Note that $\lambda_i \geq 0$, $i = 1, \ldots, \hat{n}$ and $\sum_{i=1}^{\hat{n}} \lambda_i = 1$. Since $\hat{X}_i \in \Pi$ for all i and $R \succeq 0$, we follow from (12) that $Y_R \succeq 0$, and

$$Y_R e = \sum_{i=1}^{\hat{n}} \lambda_i \hat{X}_i R e = X R e, \tag{14}$$

$$\mathrm{diag}(Y_R) = \sum_{i=1}^{\hat{n}} \lambda_i \hat{X}_i \mathrm{diag}(R) = X \mathrm{diag}(R). \tag{15}$$

In the following, we show that

$$Y_R - X R X^T \succeq 0. \tag{16}$$

Since $R \succeq 0$, we have $R = V V^T$ for some $V \in \mathrm{S}^n$. Therefore, from (13), for any $d \in \Re^n$, we have

$$\begin{aligned}
d^T X R X^T d &= \left(V^T X^T d\right)^T \left(V^T X^T d\right) = \left\|V^T X^T d\right\|_2^2 \\
&= \left\| \sum_{i=1}^{\hat{n}} \lambda_i V^T \hat{X}_i^T d \right\|_2^2 \\
&\leq \sum_{i=1}^{\hat{n}} \lambda_i \left\| V^T \hat{X}_i^T d \right\|_2^2 \\
&= \sum_{i=1}^{\hat{n}} \lambda_i \left(V^T \hat{X}_i^T d \right)^T \left(V^T \hat{X}_i^T d \right) \\
&= \sum_{i=1}^{\hat{n}} \lambda_i d^T \left(\hat{X}_i R \hat{X}_i^T \right) d = d^T Y_R d,
\end{aligned}$$

where the above inequality follows from the fact that the function $\| \cdot \|_2^2$ is convex and because $\sum_{i=1}^{\hat{n}} \lambda_i = 1$ and $\lambda_i \geq 0$, $i = 1, \ldots, \hat{n}$, while the last equality follows directly from (13). The above relation means that (16) holds true.

Now let us define

$$\bar{Y}_1 = Y_1 + Y_R, \quad \bar{Y}_2 = Y_2 + Y_R.$$

Since

$$\begin{aligned}\bar{Y}_1 - XB_1X^T &= Y_1 - X(B_1 - R)X^T + Y_R - XRX^T,\\ \bar{Y}_2 - XB_2X^T &= Y_1 - X(B_2 - R)X^T + Y_R - XRX^T,\end{aligned}$$

it follows from (7)-(11) and (14)-(16) that

$$\begin{aligned}&Y = \bar{Y}_1 - \bar{Y}_2, \quad \bar{Y}_1 - XB_1X^T \succeq 0, \quad \bar{Y}_2 - XB_2X^T \succeq 0,\\ &\mathrm{diag}\,(\bar{Y}_1) = X\mathrm{diag}\,(B_1), \quad \bar{Y}_1 e = XB_1 e,\\ &\mathrm{diag}\,(\bar{Y}_2) = X\mathrm{diag}\,(B_2), \quad Y_2 e = XB_2 e,\\ &Xe = X^T e = e, \quad X \geq 0.\end{aligned}$$

The above relation implies $Y \in \bar{\Upsilon}_1(B_1, B_2)$. This proves (6). □

From Theorem 2.5, we see that given a QAP with matrices (A, B) and a PSD matrix splitting (B_1, B_2) of B, if the matrix splitting (B_1, B_2) is redundant, then we have

$$\min_{Y \in \bar{\Upsilon}_1(B_1 - R, B_2 - R)} \mathrm{Tr}(AY) \geq \min_{Y \in \bar{\Upsilon}_1(B_1, B_2)} \mathrm{Tr}(AY). \tag{17}$$

Therefore, in order to derive a strong lower bound, a non-redundant PSD matrix splitting should be used.

We next discuss how to find a non-redundant PSD matrix splitting for a given matrix B. For this, we consider the following auxiliary problem based on the minimal trace principle

$$\begin{array}{lll}(\mathrm{MTMS-PSD}) & \min & \mathrm{Tr}(B_1)\\ & \text{s. t.} & B_1 - B_2 = B,\\ & & B_1 \succeq 0, \quad B_2 \succeq 0.\end{array}$$

It is easy to see that the above problem is strictly feasible.

For a given matrix B, let Q be an orthogonal matrix whose columns are the eigenvectors of the matrix B associated with the eigenvalues $\{\lambda_1, \cdots, \lambda_n\}$, i.e., $B = \sum_{i=1}^n \lambda_i q_i q_i^T$ where q_i is the i-th column of Q. Let us define

$$B^+ = \sum_{i:\lambda_i \geq 0} \lambda_i q_i q_i^T, \quad B^- = -\sum_{i:\lambda_i < 0} \lambda_i q_i q_i^T. \tag{18}$$

Our next result establishes the equivalence between the optimal solution to the MTMS-PSD problem and the so-called orthogonal PSD splitting introduced in [20].

Theorem 2.6. *The optimal solution to the MTMS-PSD problem can be obtained by using the eigenvalue decomposition of B. Further, the splitting (B^+, B^-) is non-redundant.*

Proof. Denote the optimal solution to the MTMS-PSD problem by (B_1^*, B_2^*). We first show $(B_1^*, B_2^*) = (B^+, B^-)$. Let P be the projection matrix defined by

$$P = \sum_{i:\lambda_i \geq 0} q_i q_i^T.$$

It follows immediately that

$$\mathrm{Tr}(B_1^*) \geq \mathrm{Tr}(B_1^* P) = \mathrm{Tr}\big(B_1^* P^2\big) = \mathrm{Tr}(P B_1^* P) \geq \mathrm{Tr}(P(B_1^* - B_2^*)P) = \mathrm{Tr}\big(B^+\big),$$

where the first inequality follows from the relation

$$\mathrm{Tr}(B_1^*(I-P)) \geq 0.$$

Similarly, one has

$$\mathrm{Tr}(B_2^*) \geq \mathrm{Tr}(B_2^*(I-P)) = \mathrm{Tr}((I-P)B_2^*(I-P)) \geq \mathrm{Tr}\big(B^-\big).$$

Therefore, we have

$$\mathrm{Tr}(B_1^*) + \mathrm{Tr}(B_2^*) \geq \mathrm{Tr}\big(B^+\big) + \mathrm{Tr}\big(B^-\big),$$

and the equality holds if and only if

$$\mathrm{Tr}(B_1^*(I-P)) = 0, \quad \mathrm{Tr}(B_2^* P) = 0. \tag{19}$$

Since all the matrices B_1^*, B_2^*, P and $I-P$ are positive semi-definite. Relation (19) holds if and only if

$$B_1^* P = P B_1^*, \quad B_2^* P = P B_2^* = 0. \tag{20}$$

It follows immediately

$$B_1^* = PBP = B^+, \quad B_2^* = -(I-P)B(I-P) = B^-.$$

It remains to show that the matrix splitting (B^+, B^-) is non-redundant. Suppose to the contrary that (B^+, B^-) is a redundant splitting of B, i.e., there exists $R \neq 0 \succeq 0$ such that

$$B_1 = B^+ - R \succeq 0, \quad B_2 = B^- - R \succeq 0, \quad B_1 - B_2 = B.$$

Then we have

$$\mathrm{Tr}\big(B^+ B^-\big) = \mathrm{Tr}((B_1 + R)(B_2 + R)) \geq \mathrm{Tr}(B_1 B_2) + \mathrm{Tr}\big(R^2\big) > 0,$$

which contradicts to the relation $\mathrm{Tr}\big(B^+ B^-\big) = 0$. Therefore, (B^+, B^-) is a non-redundant splitting of B. □

Based on Theorem 2.6, for a given matrix B, if its non-redundant splitting is unique, then the SDP relaxation based on the orthogonal PSD matrix splitting will be the strongest among all the PSD matrix splittings. However, as one can see from the following example, the non-redundant PSD matrix splitting of a matrix might not be unique.

Example 2.7. Consider the matrix

$$B = \begin{pmatrix} 0 & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix}.$$

By solving the MTMS-PSD problem with the above B, we obtain the optimal solution as follows

$$B_1^* = \begin{pmatrix} 1.0774 & 0.7887 & 1.0774 \\ 0.7887 & 0.5774 & 0.7887 \\ 1.0774 & 0.7887 & 1.0774 \end{pmatrix}, \quad B_2^* = \begin{pmatrix} 1.0774 & -0.2113 & -0.9226 \\ -0.2113 & 0.5774 & -0.2113 \\ -0.9226 & -0.2113 & 1.0774 \end{pmatrix}.$$

By Theorem 2.6, (B_1^*, B_2^*) is an orthogonal and non-redundant PSD matrix splitting of B. One can easily check that $\mathrm{Tr}(B_1^* B_2^*) = 0$.

Now, let us choose

$$B_1 = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \qquad B_2 = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}.$$

It is easy to see that (B_1, B_2) is a PSD matrix splitting of B. Since $\mathrm{Tr}(B_1 B_2) \neq 0$, by Theorem 2.6, (B_1, B_2) is not the optimal solution to the MTMS-PSD problem. We next show that (B_1, B_2) is also non-redundant. Suppose to the contrary that (B_1, B_2) is redundant, i.e., there exists $R \neq 0 \succeq 0$ satisfying

$$B_1 - R \succeq 0, \qquad B_2 - R \succeq 0.$$

Since $B_1 = E$ and $B_1 - R \succeq 0$, it must hold that $R = \alpha E$ for some $0 < \alpha \leq 1$. On the other hand, for any $0 < \alpha \leq 1$, one can easily check that the matrix $B_2 - \alpha E$ is not positive semidefinite.

The non-uniqueness of the non-redundant PSD matrix splitting for a given matrix B shown in the above example illustrates that it is nontrivial to find the strongest SDP relaxation based on matrix splitting. In the next section, we will present two other matrix splitting schemes.

3 Two Matrix Splitting Schemes based on Minimal Trace Principal

In this section, we first use the minimal trace principle to derive two matrix splitting schemes and characterize conditions under which the constructed matrix splitting is non-redundant. Then, we compare the lower bounds provided by the SDP relaxations of QAPs based on these two matrix splitting schemes. We start by stating an assumptions regarding the QAPs throughout this section.

Assumption 3.1. *At least one matrix (A or B) in the underlying QAP has zeros on its diagonal.*

It should be pointed out that the above assumption is quite reasonable and most QAP instances from the QAP library indeed satisfy such a condition. For convenience of discussion, in the remaining part of this section, we assume that the matrix A has zeros on its diagonal.

Under Assumption 3.1, we can easily show that for any diagonal matrix D, one has

$$\mathrm{Tr}\big(AXBX^T\big) = \mathrm{Tr}\big(AX(B-D)X^T\big), \quad \forall X \in \Pi. \tag{21}$$

3.1 Minimal trace one-matrix splitting

Let us first consider a special case of the MTMS-PSD problem when $B_1 = tE$ for $t \geq 0$. In such a scenario, the MTMS-PSD problem reduces to the auxiliary SDP problem considered in [20]:

$$(22) \qquad \begin{array}{ll} \min & \alpha \\ \text{s. t.} & \alpha E - B \succeq 0, \qquad \alpha \geq 0. \end{array}$$

If the problem (22) is feasible, then the optimal solution α of problem (22) is used to split the matrix B into the following form used in [17]:

$$B = \alpha E - B^-, \ B^- \succeq 0.$$

However, as pointed out in [20], the problem (22) is in general infeasible. As a remedy for such an infeasibility issue, we propose to split the matrix B into the form as follows

$$(23) \qquad B - D = \alpha E - B_2, \quad B_2 = D + \alpha E - B \succeq 0,$$

where D is a diagonal matrix to be found and α is a parameter. Similarly we call (α, D) the one-matrix splitting of the matrix B.

Like in the previous section, in order to find a non-redundant PSD matrix splitting for the matrix B or $B - D$, we apply the minimal trace principle to obtain an auxiliary problem as follows:

$$(24) \qquad \begin{array}{ll} \min\limits_{\alpha \in \Re, \ d \in \Re^n} & n\alpha + \sum\limits_{i=1}^{n} d_i \\ \text{s. t.} & \alpha E + D - B \succeq 0, \quad D = \mathrm{Diag}(d). \end{array}$$

It is easy to see that the above problem is strictly feasible.

Proposition 3.2. *Let (α, D) be the minimal trace one-matrix splitting of matrix B. Then* $\mathrm{rank}(\alpha E + D - B) < n$.

Proof. Let $B_2 = \alpha E + D - B$. Now suppose that $\mathrm{rank}(B_2) = n$, then $B_2 \succ 0$. There exists $\beta > 0$ such that $B_2 - \beta I \succeq 0$. Thus, $(\alpha, d - \beta e)$ is also a feasible solution to problem (24) with the objective value $n\alpha + (d - \beta e)^T e < n\alpha + d^T e$, contradicting the assumption that (α, d) is the solution of problem (24). Therefore, it must hold $\mathrm{rank}(B_2) < n$. □

The following well-known result for matrix product from [25] will be used in our later analysis.

Lemma 3.3. *Let $A, B \in \mathrm{S}^n$ with the eigenvalues $\lambda_i(A)$ and $\lambda_i(B)$, $i = 1, \ldots, n$ listed in nonincreasing order. Then*

$$\mathrm{Tr}(AB) \leq \sum_{i=1}^{n} \lambda_i(A)\lambda_i(B),$$

where the equality holds if and only if there is an orthogonal matrix P whose columns form a common set of eigenvectors for A and B and are ordered with respect to $\{\lambda_i(A)\}_{i=1}^n$ and $\{\lambda_i(B)\}_{i=1}^n$, such that $P^{-1}AP$ and $P^{-1}BP$ are diagonal.

Now we consider a special case of problem (24) where $D = \beta I$, i.e.,

$$(25) \qquad \min \left\{ n(\alpha + \beta) : \alpha E + \beta I - B \succeq 0, \ \ (\alpha, \beta) \in \Re^2 \right\},$$

We have

Theorem 3.4. *Suppose that the matrix B in QAPs is non-negative. Let (α, β) be the optimal solution of problem (25). Then $\alpha > 0$.*

Proof. Since (α, β) is an optimal solution of problem (25), there exists $U \in \mathrm{S}^n$ such that

$$n - \mathrm{Tr}(UE) = 0, \tag{26}$$

$$n - \mathrm{Tr}(U) = 0, \tag{27}$$

$$\mathrm{Tr}(U(\alpha E + \beta I - B)) = 0, \tag{28}$$

$$U \succeq 0, \quad \alpha E + \beta I - B \succeq 0. \tag{29}$$

From (26)-(28), we obtain directly

$$n(\alpha + \beta) = \mathrm{Tr}(UB). \tag{30}$$

From (28) and (29), we follow that

$$U(\alpha E + \beta I - B) = (\alpha E + \beta I - B)U = 0. \tag{31}$$

This implies that U and $\alpha E + \beta I - B$ can commute. By Theorem 1.3.12 in [13], U and $\alpha E + \beta I - B$ are simultaneously diagonalizable. Since $U \in \mathrm{S}^n$, $\alpha E + \beta I - B \in \mathrm{S}^n$, there is an orthogonal matrix P such that $P^{-1}UP$ and $P^{-1}(\alpha E + \beta I - B)P$ are diagonal. So, we have

$$\mathrm{Tr}(U(\alpha E + \beta I - B)) = \sum_{i=1}^{n} \lambda_i(U)\lambda_i(\alpha E + \beta I - B) = 0,$$

which in turn by (29) implies that

$$\lambda_i(U)\lambda_i(\alpha E + \beta I - B) = 0, \ i = 1, \ldots, n. \tag{32}$$

By Proposition 3.2, $s = \mathrm{rank}(\alpha E + \beta I - B) < n$. Since $\alpha E + \beta I - B \succeq 0$, we assume that $\lambda_i(\alpha E + \beta I - B) > 0$, $i = 1, \ldots, s$. The above equality (32) then yields $\lambda_i(U) = 0$, $i = 1, \ldots, s$.

We now prove $UE \neq EU$. Suppose to the contrary that $UE = EU$. By Theorem 1.3.12 in [13], U and E are simultaneously diagonalizeable. Let

$$\lambda_1(U) = \ldots = \lambda_s(U) = 0 < \lambda_{s+1}(U) \leq \ldots \leq \lambda_n(U). \tag{33}$$

Note that the eigenvalues of E are $0, \ldots, 0, n$. Therefore, we have

$$\mathrm{Tr}(UE) = n\lambda_n(U),$$

which by (26) implies $\lambda_n(U) = 1$. Hence, we infer from (33) that

$$\mathrm{Tr}(U) = \sum_{i=1}^{n} \lambda_i(U) \leq n - s < n,$$

this contradicts (27).

Because $UE \neq EU$, from (31) we obtain $UB \neq BU$. Since $U \in \mathrm{S}^n$ and $B \in \mathrm{S}^n$, by Theorem 1.3.12 in [13], U and B are not simultaneously diagonalizable. Now using Lemma 3.3, we have

$$\mathrm{Tr}(UB) < \sum_{i=1}^{n} \lambda_i(U)\lambda_i(B),$$

which, together with (30), yields

$$n(\alpha+\beta) < \sum_{i=1}^{n} \lambda_i(U)\lambda_i(B). \tag{34}$$

Let $\lambda_{\max}(B)$ be the largest eigenvalue of B. Note that $\sum_{i=1}^{n} \lambda_i(U) = \mathrm{Tr}(U) = n$. Also, $\lambda_i(U) \geq 0$ for all i since $U \succeq 0$. It then follows from (34) that

$$\alpha+\beta < \lambda_{\max}(B). \tag{35}$$

On the other hand, from (29), we have

$$B - \alpha(E-I) - (\alpha+\beta)I \preceq 0.$$

This means that

$$\alpha+\beta \geq \lambda_{\max}(B-\alpha(E-I)). \tag{36}$$

If $\alpha = 0$, then the combination of (35) and (36) leads to a contradiction.

If $\alpha < 0$. Let $\rho(B)$ be the spectral radius of B. Since $B \in \mathrm{S}^n$ is non-negative, by Theorem 8.3.1 in [13], then $\rho(B)$ is an eigenvalue of B and there exists nontrivial $\hat{x} \geq 0 \in \Re^n$ such that $B\hat{x} = \rho(B)\hat{x}$. Without loss of generality, we can further assume that $\|\hat{x}\|_2 = 1$. Thus we have $\hat{x}^T B\hat{x} = \rho(B)$. Since $\hat{x} \geq 0$, it holds $\hat{x}^T(E-I)\hat{x} \geq 0$. It follows from (36) that

$$\begin{aligned}
\alpha+\beta &\geq \lambda_{\max}(B-\alpha(E-I)) \\
&= \max\left\{x^T(B-\alpha(E-I))x : x^Tx = 1\right\} \\
&\geq \hat{x}^T(B-\alpha(E-I))\hat{x} \\
&\geq \hat{x}^T B\hat{x} \\
&= \rho(B) \\
&\geq \lambda_{\max}(B),
\end{aligned}$$

which contradicts to (35). Therefore, we can conclude $\alpha > 0$. This finishes the proof of the theorem. □

Similarly, we have the following result.

Theorem 3.5. *Let (α,β) be the optimal solution of problem (25). Then we have*

(i) $(\alpha E+\beta I, \alpha E+\beta I - B)$ is a non-redundant PSD matrix splitting of B if $\beta \leq 0$;

(ii) If $\beta > 0$, then $(\alpha E+\beta I, \alpha E+\beta I - B)$ is a redundant PSD matrix splitting of B.

Proof. We first consider statement (i). By Theorem 3.4, $\alpha > 0$. If $\beta < 0$, the matrix $\alpha E+\beta I$ is not positive semidefinite. Therefore, $(\alpha E+\beta I, \alpha E+\beta I-B)$ is a non-redundant PSD matrix splitting of B. It remains to prove the statement for the case $\beta = 0$, which implies $B_1 = \alpha E, B_2 = \alpha E - B$. It is easy to see that (B_1, B_2) is a PSD matrix splitting of $B - \beta I$. We claim that (B_1, B_2) is non-redundant. Suppose to the contrary that (B_1, B_2) is redundant, i.e., there exists nonzero matrix $R \succeq 0$ satisfying

$$B_1 - R \succeq 0, \quad B_2 - R \succeq 0.$$

Since $B_1 = \alpha E$, $\alpha > 0$ and $B_1 - R \succeq 0$, it must hold that $R = \tau E$ for some $0 < \tau \leq \alpha$. Therefore,

$$B_2 - R = (\alpha - \tau)E - B \succeq 0.$$

This implies that $(\alpha - \tau, 0)$ is a feasible solution of problem (MTMS-ONE). Note that $n(\alpha - \tau) < n\alpha$. This contradicts to the optimality of $(\alpha, 0)$ with respect to problem (25). This proves statement (i).

Now we turn to statement (ii). Since $\beta > 0$ and $\alpha > 0$ (by Theorem 3.4), we have $\alpha E + \beta I \succ 0$. Because $B = (\alpha E + \beta I) - (\alpha E + \beta I - B)$, and $\alpha E + \beta I - B \succeq 0$, $(\alpha E + \beta I, \alpha E + \beta I - B)$ is a PSD matrix splitting of B. Now let us choose a $\eta \in (0, 1)$ satisfying

$$\lambda_{\max}\left(\eta(\alpha E + \beta I - B)\right) < \beta.$$

Let $R = \eta(\alpha E + \beta I - B) \succeq 0$. It is easy to show that $\alpha E + \beta I - R \succeq 0$ and $\alpha E + \beta I - B - R \succeq 0$. Therefore, the matrix splitting $(\alpha E + \beta I, \alpha E + \beta I - B)$ is redundant. $\square$

Theorem 3.5 implies that if problem (25) has an optimal solution (α, β) with $\beta > 0$, then the resulting SDP relaxation can be further improved by using a non-redundant PSD splitting of B. When $\beta \leq 0$, the one-matrix splitting might be a very good choice due to the simplicity of the resulting SDP relaxation model. We also point out that when B is the Hamming distance matrix of the hypercube in $\mathfrak{R}^m$, as proved in [17], the one-matrix splitting based on minimal trace principle is also the orthogonal PSD splitting of B. In such a case, the optimal solution to problem (25) is $(\alpha^*, \beta^*) = (\frac{m}{2}, 0)$.

In our experiments, we also observe that for some QAP instances such as Tai20b, Tai25b, Tai35b, Tai40b and Tai50b, problem (25) has an optimal solution with $\beta < 0$ as listed in Table 1. We can further check from Table 3 and Table 4 of Section 5 that for these QAP instances, the SDP relaxation based on the one-matrix splitting scheme can provide a stronger lower bound than that based on the orthogonal PSD matrix splitting scheme.

Table 1: Optimal solution (α, β) of problem (25)

Prob.	α	β
Tai20b	420.4951	-2.5025
Tai25b	558.5071	-2.5238
Tai35b	584.1755	-2.0483
Tai40b	797.8480	-3.5505
Tai50b	969.1780	-5.2837

3.2 Minimal trace sum-matrix splitting

In this subsection, we combine the minimal trace principle and the so-called sum-matrix to construct a non-redundant matrix splitting for a given matrix B. First we recall the following definition [3].

Definition 3.6. *A matrix M is called a sum-matrix if*

$$M = ue^T + eu^T \tag{37}$$

for some $u \in \mathrm{R}^n$. The sum-matrix has the following property:

$$X(ue^T + eu^T)X^T = Xue^T + eu^T X^T, \quad \forall X \in \Omega, \tag{38}$$

where $\Omega = \{X \in \Re^{n\times n} : Xe = X^T e = e\}$.

The sum-matrix has been used to improve the GLB and eigenvalue bound for QAPs as the reduction method in the literature [3, 6, 10, 23]. In what follows we use the sum-matrix to construct a non-redundant matrix splitting framework. Based on relation (21), we propose to split the matrix B into the following form

$$B - D = ue^T + eu^T - B_2, \quad B_2 \succeq 0, \quad D = \mathrm{Diag}(d), \tag{39}$$

where $d \in \mathrm{R}^n$ and $u \in \mathrm{R}^n$ are vectors to be found. Similarly, we call that (u, D) is a sum-matrix splitting of the matrix B if there exists (u, D) satisfying (39). Like in the last subsection, we use the minimal trace principle to find a non-redundant sum-matrix splitting of the matrix B as follows.

$$\begin{array}{lll} \min\limits_{u\in\Re^n, d\in\Re^n} & e^T(2u + d) \\ \text{s. t.} & ue^T + eu^T + D - B \succeq 0, \quad D = \mathrm{Diag}(d). \end{array} \tag{40}$$

It is easy to see that the above problem is strictly feasible. It should be pointed out that for simplicity of the model, we can also impose the constraint that $D = \beta I$ for some parameter $\beta \in \Re$. It is worthy mentioning that the sum-matrix splitting (u, D) of B includes the one-matrix splitting (α, D) as a special case where $u = \frac{\alpha}{2}e$ for some $\alpha \in \Re$.

Similar to the one-matrix splitting case, we have the following result.

Proposition 3.7. *Let (u, d) be the solution of the problem (40) and $B_2 = ue^T + eu^T + D - B$. Then rank$(B_2) < n$.*

Proof. The proof is similar to that of Proposition 3.2 and thus the details are omitted. □

The above proposition forms the basis of a new implementation of the relaxed SDP model to be discussed in later sections.

3.3 Relations between the lower bounds

In this subsection, we compare the two lower bounds provided by the SDP relaxations based on the one-matrix splitting and the sum-matrix splitting described in the previous subsections.

Let (α, D) and (u, D) be respectively a minimal trace one-matrix splitting and sum-matrix splitting of B. Then we can derive the following two SDP relaxations of QAPs

$$\mu_2(\alpha, D) = \min_{Y\in\bar{\mathrm{Y}}_2(\alpha,D)} \alpha\mathrm{Tr}(AE) - \mathrm{Tr}(AY), \tag{41}$$

$$\mu_3(u, D) = \min_{(X,Y)\in\bar{\mathrm{Y}}_3(u,D)} \mathrm{Tr}\big(AXue^T + Aeu^T X^T\big) - \mathrm{Tr}(AY), \tag{42}$$

where the feasible sets $\bar{\mathrm{Y}}_2(\alpha, D)$ and $\bar{\mathrm{Y}}_3(\alpha, D)$ are respectively defined by

$$\bar{\mathrm{Y}}_2(\alpha, D) = \left\{ \begin{array}{c} Y \in \mathcal{S}^n, \\ X \in \Re^{n\times n} \end{array} \;\middle|\; \begin{array}{c} Y - \alpha E - X(D-B)X^T \succeq 0, \\ Ye = n\alpha e + X(D-B)e, \\ \mathrm{diag}\,(Y) = \alpha e + X\mathrm{diag}\,(D-B), \\ Xe = X^T e = e, \quad X \geq 0 \end{array} \right\}, \tag{43}$$

$$\bar{\mathrm{Y}}_3(u, D) = \left\{ \begin{array}{c} Y \in \mathcal{S}^n, \\ X \in \Re^{n\times n} \end{array} \;\middle|\; \begin{array}{c} Y - Xue^T - eu^T X^T + X(B-D)X^T \succeq 0, \\ Ye = nXu + eu^T e - X(B-D)e, \\ \mathrm{diag}\,(Y) = 2Xu - X\mathrm{diag}\,(B-D), \\ Xe = X^T e = e, \quad X \geq 0 \end{array} \right\}. \tag{44}$$

For simplicity of discussion, we concentrate only on a special case of problem (40) with $D = \beta I$ for $\beta \in \Re$ defined by

$$\begin{array}{rl} \min\limits_{u\in\Re^n, \beta\in\Re} & 2e^T u + n\beta \\ \text{s. t.} & ue^T + eu^T + \beta I - B \succeq 0. \end{array} \tag{45}$$

Lemma 3.8. *Suppose that $(\bar{\alpha}, \bar{\beta})$ and $(\hat{u}, \hat{\beta})$ are the optimal solution of problems (25) and (45), respectively. Then $\bar{\beta} \geq \hat{\beta}$.*

Proof. Denote (u, β) any feasible solution to problem (45). Let define

$$\alpha = \frac{2u^T e}{n}, \quad v = u - \frac{\alpha}{2} e.$$

It follows immediately

$$u = \frac{\alpha}{2} e + v, \quad v^T e = 0.$$

Using the above notation, we can rewrite problem (45) as

$$\begin{array}{rl} \min\limits_{v\in\Re^n, \beta\in\Re} & n\alpha + n\beta \\ \text{s. t.} & \alpha E + ve^T + ev^T + \beta I - B \succeq 0; \\ & e^T v = 0. \end{array} \tag{46}$$

We next show that the optimal solution to the above problem can be obtained explicitly. Denote the optimal solution of problem (46) by $(\hat{\alpha}, \hat{\beta})$ and $P = I - \frac{E}{n}$. From the constraint $e^T v = 0$ we obtain

$$P(\hat{\alpha} E + ve^T + ev^T + \hat{\beta} I - B)P = \hat{\beta} P - PBP \succeq 0,$$

which implies

$$\hat{\beta} \geq \lambda_{\max}(PBP).$$

Here $\lambda_{\max}(PBP)$ denotes the largest eigenvalue of the matrix PBP in the null space of e. Similarly, we have

$$(I-P)(\hat{\alpha} E + ve^T + ev^T + \hat{\beta} I - B)(I-P) = \hat{\alpha} E + \frac{\hat{\beta}}{n} E - \frac{e^T Be}{n^2} E \succeq 0,$$

which implies

$$n\hat{\alpha} + \hat{\beta} \geq \frac{e^T Be}{n}.$$

It follows that

$$\hat{\alpha} + \hat{\beta} \geq \frac{e^T Be}{n^2} + \frac{(n-1)\hat{\beta}}{n} \geq \frac{e^T Be}{n^2} + \frac{(n-1)}{n}\lambda_{\max}(PBP).$$

Now let us choose

$$v = \frac{e^T Be}{n} e - Be, \quad \beta = \lambda_{\max}(PBP), \quad \alpha = \frac{e^T Be}{n^2} - \frac{\beta}{n}.$$

One can easily verify that (α, β, v) satisfy all the constraints in problem (46). Therefore, we can conclude that at the optimal solution of problem (46), it must hold

$$\hat{\alpha} = \frac{e^T Be}{n^2} - \frac{1}{n}\lambda_{\max}(PBP), \quad \hat{\beta} = \lambda_{\max}(PBP).$$

On the other hand, if $(\bar{\alpha}, \bar{\beta})$ is the optimal solution to problem (25), then by following a similar process, one can show that

$$\bar{\beta} \geq \lambda_{\max}(PBP) = \hat{\beta}.$$

The proof of the lemma is finished. □

Based on Lemma 3.8, we can establish the following result regarding the two lower bounds $\mu_2(\alpha, \bar{\beta} I)$ and $\mu_3(u, \hat{\beta} I)$.

Theorem 3.9. *Assume that $(\alpha, \bar{\beta} I)$ and $(u, \hat{\beta} I)$ are the minimal trace one-matrix splitting and sum-matrix splitting of B, respectively. Then we have*

$$\mu_3(u, \hat{\beta} I) \geq \mu_2(\alpha, \bar{\beta} I). \tag{47}$$

Proof. Let (X, Y) be the optimal solution of the problem (42). Then we have

$$Y - Xue^T - eu^T X^T - X(\hat{\beta} I - B)X^T \succeq 0, \tag{48}$$

$$Ye = nXu + eu^T e + X(\hat{\beta} I - B)e, \tag{49}$$

$$\mathrm{diag}\,(Y) = 2Xu + X\mathrm{diag}\,(\hat{\beta} I - B), \tag{50}$$

$$Xe = X^T e = e, \quad X \geq 0, \tag{51}$$

and

$$\mu_3(u, \hat{\beta} I) = \mathrm{Tr}\big(AXue^T + Aeu^T X^T\big) - \mathrm{Tr}(AY). \tag{52}$$

Since X is a $n \times n$ doubly stochastic matrix, similar to the proof of Theorem 2.5, we can infer that there exist $\hat{n} \in \mathrm{N}$, $\hat{X}_i \in \Pi$ and $\lambda_i \in \Re$, $i = 1, \ldots, \hat{n}$, with $\lambda_i \geq 0$ for all i and $\sum_{i=1}^{\hat{n}} \lambda_i = 1$, such that

$$X = \sum_{i=1}^{\hat{n}} \lambda_i \hat{X}_i,$$

from which, we can easily infer that

$$\operatorname{diag}(Xue^T) = \sum_{i=1}^{\hat{n}} \lambda_i \operatorname{diag}(\hat{X}_i ue^T) = \sum_{i=1}^{\hat{n}} \lambda_i \hat{X}_i \operatorname{diag}(ue^T) = \sum_{i=1}^{\hat{n}} \lambda_i \hat{X}_i u = Xu,$$

which, together with $eu^T X^T = (Xue^T)^T$, implies that

$$\operatorname{diag}(eu^T X^T) = \operatorname{diag}(Xue^T) = Xu. \tag{53}$$

Since X is a doubly stochastic matrix, we have

$$I - XX^T \succeq 0. \tag{54}$$

Let us choose

$$\hat{Y} = Y - Xue^T - eu^T X^T + \alpha E + (\bar{\beta} - \hat{\beta})I. \tag{55}$$

Note that

$$\begin{aligned} &\hat{Y} - \alpha E - X(\bar{\beta} I - B)X^T \\ &= Y - Xue^T - eu^T X^T - X(\hat{\beta} I - B)X^T + (\bar{\beta} - \hat{\beta})(I - XX^T). \end{aligned}$$

By Lemma 3.8, $\bar{\beta} - \hat{\beta} \geq 0$. We then follow immediately from (48)-(51), (53) and (54) that

$$\begin{aligned} &\hat{Y} - \alpha E - X(\bar{\beta} I - B)X^T \succeq 0, \\ &\hat{Y} e = n\alpha e + X(\bar{\beta} I - B)e, \\ &\operatorname{diag}(\hat{Y}) = \alpha e + X \operatorname{diag}(\bar{\beta} I - B). \end{aligned}$$

These, together with (51), imply that $\hat{Y} \in \bar{\mathrm{Y}}_2(\alpha, \bar{\beta} I)$, thus

$$\alpha \operatorname{Tr}(AE) - \operatorname{Tr}\left(A\hat{Y}\right) \geq \mu_2(\alpha, \bar{\beta} I). \tag{56}$$

On the other hand, under Assumption 3.1, we can deduce from (55) that

$$\alpha \operatorname{Tr}(AE) - \operatorname{Tr}\left(A\hat{Y}\right) = \operatorname{Tr}\left(AXue^T + Aeu^T X^T\right) - \operatorname{Tr}(AY),$$

which, together with (52) and (56), implies that

$$\mu_3(u, \hat{\beta} I) \geq \mu_2(\alpha, \bar{\beta} I),$$

this proves (47). □

Theorem 3.9 shows that under certain conditions, the SDP relaxation (42) based on the sum-matrix splitting is at least as good as the SDP relaxation (41) based on the one-matrix splitting. However, in our numerical experiments, we have observed that in most cases, we have $\mu_3(u, D) > \mu_2(\alpha, D)$. Theorem 3.9 provides a partial interpretation for such a phenomenon. It should also be pointed out that, as illustrated by the numerical results in Section 5, there is no dominative relation between the bounds derived from the three different matrix splitting schemes described in this work.

4 SDP relaxations of QAPs based on minimal trace matrix splitting

In this section, we present the SDP relaxation models of QAPs based on the three matrix splitting schemes discussed in Section 2 and 3 using the framework introduced in [20], which combine a technique to reduce the dimension of PSD constraints.

We first present the SDP relaxation model of QAP derived from the so-called minimal trace PSD matrix splitting (denoted by SDRMS-PSD). Let (B_1, B_2) be a minimal trace matrix splitting of the matrix B. Since (B_1, B_2) is the orthogonal PSD splitting of B, we have $\mathrm{rank}(B_i) < n$, $i = 1, 2$. Because $B_1 \succeq 0$ and $B_2 \succeq 0$, we have $B_i = \hat{B}_i^T \hat{B}_i$ for some $\hat{B}_i \in \Re^{m_i \times n}$, $i = 1, 2$. Based on the well-known Schur complement lemma, the quadratic PSD constraints

$$Y_i - XB_iX^T \succeq 0, \quad i = 1, 2,$$

can be equivalently replaced by the PSD constraints of smaller scale

$$\begin{pmatrix} I_{m_i \times m_i} & \hat{B}_i X^T \\ X\hat{B}_i^T & Y_i \end{pmatrix}_{(m_i+n)\times(m_i+n)} \succeq 0, \quad i = 1, 2. \tag{57}$$

Moreover, for $i = 1, 2$, one way to obtain a decomposition $B_i = \hat{B}_i^T \hat{B}_i$ is to let $\hat{B}_i = \hat{\Lambda}_i \hat{V}_i^T$, where $\hat{\Lambda}_i$ is a $m_i \times m_i$ diagonal matrix with the square roots of the m_i non-zero eigenvalues of matrix $\hat{B}_i$ as its diagonal elements, and $\hat{V}_i$ is a $n \times m_i$ matrix with eigenvectors associated with the non-zero eigenvalues as its columns in corresponding order.

Let $B_s = B_1 + B_2$. The SDP relaxation model of QAP based on minimal trace PSD matrix splitting is identical to the model introduced in [20]. For self-completeness, this model is described as follows:

$$\min \quad \mathrm{Tr}(AY) \tag{58}$$

$$s.t. \quad Y = Y_1 - Y_2, \quad Y_s = Y_1 + Y_2; \tag{59}$$

$$\begin{pmatrix} I_{m_1 \times m_1} & \hat{B}_1 X^T \\ X\hat{B}_1 & Y_1 \end{pmatrix} \succeq 0, \quad \begin{pmatrix} I_{m_2 \times m_2} & \hat{B}_2 X^T \\ X\hat{B}_2 & Y_2 \end{pmatrix} \succeq 0; \tag{60}$$

$$\mathrm{diag}\,(Y_1) = X\mathrm{diag}\,(B_1), \quad Y_1 e = XB_1 e; \tag{61}$$

$$\mathrm{diag}\,(Y_2) = X\mathrm{diag}\,(B_2), \quad Y_2 e = XB_2 e; \tag{62}$$

$$(X\min([B_1]_{off}))_i \le [Y_1]_{i,j} \le (X\max([B_1]_{off}))_i, \quad \forall i \neq j; \tag{63}$$

$$(X\min([B_2]_{off}))_i \le [Y_2]_{i,j} \le (X\max([B_2]_{off}))_i, \quad \forall i \neq j; \tag{64}$$

$$(X\min([B]_{off}))_i \le [Y]_{ij} \le (X\max([B]_{off}))_i, \quad \forall i \neq j; \tag{65}$$

$$(X\min([B_s]_{off}))_i \le [Y_s]_{ij} \le (X\max([B_s]_{off}))_i, \quad \forall i \neq j; \tag{66}$$

$$\mathcal{L}_2(Y_1) \le X\mathcal{L}_2(B_1), \quad \mathcal{L}_2(Y_2) \le X\mathcal{L}_2(B_2); \tag{67}$$

$$\mathcal{L}_2(Y) \le X\mathcal{L}_2(B), \quad \mathcal{L}_2(Y_s) \le X\mathcal{L}_2(B_s); \tag{68}$$

$$X \ge 0, \quad Xe = X^T e = e. \tag{69}$$

Next, we present the SDP relaxation model of QAPs based on minimal trace sum-matrix splitting (denoted by SDRMS-SUM). Let (u, d) be the optimal solution of the above MTMS-SUM problem, we obtain a minimal trace sum-matrix splitting of the matrix B, i.e.,

$$B_2 = ue^T + eu^T + D - B \succeq 0.$$

Let $B_s = ue^T + eu^T + \text{diag}\,(d) + B_2$. By Proposition 3.7, $m = \text{rank}(B_2) < n$. Let $\hat{B}_2$ be a $m \times n$ matrix such that $B_2 = \hat{B}_2^T \hat{B}_2$.

We thus obtain the SDRMS-SUM as follows

$$\begin{aligned}
(70)\qquad & \min \quad \text{Tr}(AY) \\
(71)\qquad & \text{s.t.} \quad Y = Xue^T + eu^T X^T + \text{diag}\,(Xd) - Y_2, \\
(72)\qquad & Y_s = Xue^T + eu^T X^T + \text{diag}\,(Xd) + Y_2, \\
(73)\qquad & \begin{pmatrix} I_{m\times m} & \hat{B}_2 X^T \\ X\hat{B}_2^T & Y_2 \end{pmatrix} \succeq 0, \\
(74)\qquad & \text{diag}\,(Y_2) = X\text{diag}\,(B_2), \quad Y_2 e = XB_2 e, \\
(75)\qquad & (X \min([B_2]_{off}))_i \le [Y_2]_{i,j} \le (X \max([B_2]_{off}))_i, \quad \forall i \ne j, \\
(76)\qquad & (X \min([B]_{off}))_i \le [Y]_{i,j} \le (X \max([B]_{off}))_i, \quad \forall i \ne j, \\
(77)\qquad & (X \min([B_s]_{off}))_i \le [Y_s]_{i,j} \le (X \max([B_s]_{off}))_i, \quad \forall i \ne j, \\
(78)\qquad & \mathcal{L}_2(Y_2) \le X\mathcal{L}_2(B_2), \mathcal{L}_2(Y) \le X\mathcal{L}_2(B), \mathcal{L}_2(Y_s) \le X\mathcal{L}_2(B_s), \\
(79)\qquad & X \ge 0, \quad Xe = X^T e = e.
\end{aligned}$$

Finally, the SDP relaxation of QAP based on minimal trace one-matrix splitting (denoted by SDRMS-ONE) discussed in the previous section is a variant of the models introduced in [17, 20]. Let (α, β) be the solution of the problem (MTMS-ONE). Then $B_2 = \alpha E + \beta I - B \succeq 0$. By Proposition 3.2, $m = \text{rank}(B_2) < n$. Let $\hat{B}_2$ be a $m \times n$ matrix such that $B_2 = \hat{B}_2^T \hat{B}_2$. Denote $B_s = \alpha E + \beta I + B_2$. We then have the SDRMS-ONE as follows:

$$\begin{aligned}
(80)\qquad & \min \quad \alpha\text{Tr}(AE) - \text{Tr}(AY) \\
(81)\qquad & \text{s.t.} \quad Y_s = \alpha E + \beta I + Y, \\
(82)\qquad & \begin{pmatrix} I_{m\times m} & \hat{B}_2 X^T \\ X\hat{B}_2^T & Y \end{pmatrix} \succeq 0, \\
(83)\qquad & \text{diag}\,(Y) = X\text{diag}\,(B_2), \quad Ye = XB_2 e, \\
(84)\qquad & (X \min([B_2]_{off}))_i \le [Y]_{i,j} \le (X \max([B_2]_{off}))_i, \ \forall i \ne j, \\
(85)\qquad & \mathcal{L}_2(Y - \alpha E - \beta I) \le X\mathcal{L}_2(B), \mathcal{L}_2(Y_s) \le X\mathcal{L}_2(B_s), \\
(86)\qquad & X \ge 0, \quad Xe = X^T e = e.
\end{aligned}$$

5 Numerical Experiments

In this section, we report some numerical results of the relaxation model based on nonredundant matrix splittings. As the comparison of the SDRMS-SVD and the other existing bounds has already been reported in our earlier work [20], we only focus on the comparison of the SDP relaxation models based on the three different matrix splitting schemes - SDRMS-SUM, SDRMS-SVD and SDRMS-ONE (The readers may refer to Section 4 for details of these three relaxation models). While the SDRMS-SVD is identical to the F-SVD model used in [20], we remind the readers that the SDRMS-ONE is different from the relaxation models used in [17] in terms of the cuts and constraints. Of course, combining the constraints from the models used in [17] will strengthen the SDRMS-ONE bound, but we found those improvements are usually associated with the particular instances and thus might not be substantial for generic QAPs. On the other hand, it may conceal the computational benefits of the SDRMS-ONE bound. The SDRMS-SUM bound is derived by applying the relaxation framework introduced in [20] to the new sum-matrix splitting scheme. As QAP(A,B) is equivalent to QAP(B,A), we compute the lower bounds for both orderings of the A, B matrices and report the stronger one only for all the three models.

In our experiments, all the problems were solved in Matlab R2009b on a 3.33GHz Intel Core 2 Duo with 8GB memory. For QAPs of small and median sizes ($n \leq 70$), the SDP relaxation problems were automatically generated by CVX 1.2 [11] and solved by the SDP solver SDPT3 [26] (see Table 3 and Table 4); For QAPs of large sizes ($n > 70$), the large-scale SDP relaxation problems were solved using the new SDP solver - SDPNAL [27] and the input data was manually created on our own in order to control its structure (see Table 5). As the SDPNAL cannot handle SOCP constraints at the moment, the SOCP constraints in our models are omitted for the large QAP instances. In our numerical experiments, SDPNAL usually stops at an approximate solution, in such a case, we use the procedure described in [14] to find a rigorous bound for our relaxation model. In all the tables, the relative gap is computed by

$$R_{gap} = 1 - \frac{\text{Lower bound}}{\text{Optimal or best known feasible objective value}}$$

and listed in column R_{gap} and the CPU time (in seconds) to compute the bound in listed in column 'CPU'. For simple comparison, we use the bold font to highlight the strongest of the three bounds. We note that for several medium and large instances, the SDRMS-SUM bounds have exceeded the best-known bounds reported in QAPLIB. We list those bounds in a separate table (Table 6) for the convenience of reference.

For the SDRMS-ONE model, we also report the matrix splitting parameters α, β for the corresponding ordering in the corresponding columns. For the QAP instances that associated with a Hamming or Manhattan distance matrix, the bounds computed by splitting the distance matrices are always better than the one based on the non-distance matrix. This confirms the results in [17] from a different perspective. (see Tables 3, 4 and 5). The SDRMS-ONE bounds may be stronger than the SDRMS-SVD if the matrix splitting parameter $\beta \leq 0$ because the matrix splitting $(\alpha E + \beta I, \alpha E + \beta I - B)$ is a non-redundant matrix splitting of matrix B (see Tai20b, Tai25b in Table 3, Tai35b, Tai40b, Tai50b, Ste36c in Table 4 and Tai80b in Table 5). In some cases, the SDRMS-ONE bounds may be stronger than the SDRMS-SVD even if $\beta > 0$ (see Tai12b and Tai60b in Tables 3 and 4). This is because a new non-redundant matrix splitting $(\alpha E + \beta I - R, \alpha E + \beta I - B - R)$ can be obtained by solving the following SDP

$$\begin{array}{ll} \max & \mathrm{Tr}(R) \\ \text{s. t.} & R \succeq 0,\ \alpha E + \beta I - R \succeq 0, \\ & \alpha E + \beta I - B - R \succeq 0. \end{array}$$

For instances Tai12b and Tai60b, their SDRMS-ONE bounds can thus be improved by using the new non-redundant matrix splitting according to Theorem 2.5. But the improvements of the bounds are marginal as one can see from Table 2 because β is very small (which shows the R-redundant matrix splitting is actually very 'close' to its corresponding non-redundant matrix splitting).

For all the QAP instances tested, SDRMS-SUM bounds are always stronger than SDRMS-ONE (see Tables 3, 4 and 5). Theorem 3.9 provides a partial interpretation for such a phenomena. For most QAP instances, SDRMS-SUM bounds are stronger than the

	OPT/Feas	SDRMS-SVD	SDRMS-ONE	Improved bounds
Tai12b	39464925	28523049	28863106	28957953
Tai60b	608215054	494775609	515731315	515943103

Table 2: Improvd bounds using non-redundant matrix splitting

SDRMS-SVD bounds (see Tables 3 and 4). This is because the sum-matrix splitting is not only non-redundant, but also one part in the split form can be relaxed to linear assignment problem by using the properties of the sum-matrix. We note there is also one exception: the TaiXXc instances (see Tai64c in Table 4) where the SDRMS-SVD bound is stronger than the SDRMS-SUM bound. This is possibly due to the fact that the matrix in the TaiXXc has a very specific sparse block structure and the orthogonal PSD matrix splitting can reserve such a desirable structure, while such a structure can not be reserved if the sum matrix splitting is used. The same reasoning can also be used to explain the SDRMS-ONE bounds for TaiXXc instances (see the α, β values for Tai64c in Table 4).

In terms of computation time, we note that for small and medium scale instances, the SDRMS-SVD model is the most expensive, while the SDRMS-ONE model is the cheapest. This is not surprising due to their model complexities. Overall, SDRMS-SUM is usually preferred to SDRMS-SVD and SDRMS-ONE considering the quality of the bounds and the complexity of the model.

Table 5 has shown that SDPNAL is an very effective SDP solver for large scale SDP problems. Although, it cannot provide an exact solution to the SDP problem as SDPT3 does, the accuracy level is good enough for our purpose of estimating the lower bounds. The tightest bound of the three models are not highlighted because the relative relation can easily be affected by the accuracy level of the approximate solution found by SDPNAL with different parameters.

6 Conclusions

In this paper, we considered the issue of how to choose an appropriate matrix splitting scheme so that the resulting SDP relaxation for QAPs can provide a strong lower bound. To obtain such a desirable relaxation, we introduced the notion of redundant and non-redundant matrix splitting and showed that for every redundant splitting, there is a corresponding non-redundant splitting whose resulting SDP relaxation can provide a stronger bound. To find a non-redundant matrix splitting, we proposed to solve some auxiliary SDP problems. The properties of the optimal solutions to these SDP problems were investigated. These explored properties not only help to select the matrix splitting scheme, but also lead to a more concise and effective implementation of the relaxation model.

A new SDP relaxation for QAPs based on the sum matrix and the minimal trace principle was derived. It was shown that in special cases, the new SDP relaxation can provide a stronger bound than the one from the one-matrix splitting. Numerical results also indicates that for most tested instances, the new SDP relaxation can provide stronger bounds than the ones based on two other matrix splitting schemes.

On the other hand, we point out that although in this paper we have presented several ways to select a non-redundant PSD matrix splitting scheme to construct a strong SDP relaxation, it still remains open how to find the strongest SDP relaxation based on matrix splitting. Such a difficulty is possibly due to the multiplicity of the non-redundant splitting

	SDRMS-SUM		SDRMS-SVD		SDRMS-ONE			
Prob.	R_{gap}	CPU	R_{gap}	CPU	R_{gap}	CPU	α	β
Chr12a	**11.26%**	7	11.77%	6	66.80%	5	42.5	86.0
Chr12b	25.21%	6	**17.63%**	4	57.90%	4	42.5	86.0
Chr12c	**11.96%**	6	12.60%	7	62.51%	5	42.5	86.0
Chr15a	24.93%	9	**22.25%**	11	80.34%	7	44.2	134.7
Chr15b	36.18%	10	**35.48%**	11	81.26%	8	44.2	134.7
Chr15c	**7.54%**	11	8.14%	12	73.14%	9	44.2	134.7
Had12	**1.91%**	5	3.08%	6	3.36%	4	4	0
Had14	**1.79%**	7	2.86%	9	3.06%	5	5	0
Had16	**2.62%**	11	3.25%	11	3.63%	6	5	0
Had18	**2.58%**	13	3.29%	16	3.56%	9	6	0
Had20	**2.18%**	19	3.02%	22	3.43%	11	6.5	0
Kra30a	**16.80%**	87	16.86%	122	30.47%	42	207.5	0
Kra30b	**17.71%**	74	17.79%	149	32.39%	41	207.5	0
Nug12	**9.85%**	4	10.28%	6	10.95%	3	2.5	0
Nug14	**7.00%**	7	7.30%	7	7.43%	4	3	0
Nug15	**7.77%**	8	8.00%	9	8.16%	4	3	0
Nug16a	**7.19%**	9	8.28%	10	8.45%	5	3.5	0
Nug16b	**9.01%**	8	9.53%	9	10.25%	5	3	0
Nug17	**9.10%**	11	9.33%	11	9.70%	6	3.5	0
Nug18	**9.27%**	11	9.52%	13	9.78%	6	3.5	0
Nug20	**9.15%**	16	9.46%	19	9.72%	8	3.5	0
Nug21	**9.51%**	19	9.91%	21	10.39%	10	4	0
Nug22	**8.87%**	20	9.31%	49	9.87%	13	5.5	0
Nug24	**9.00%**	28	9.43%	31	9.77%	15	4	0
Nug25	**9.30%**	27	9.45%	37	9.82%	13	4	0
Nug27	**8.21%**	45	8.68%	54	17.18%	30	5	0
Nug28	**8.53%**	47	8.87%	71	18.09%	30	4.5	0
Nug30	**8.54%**	63	8.70%	88	9.05%	35	4.5	0
Rou12	13.54%	6	**11.48%**	8	14.52%	4	50.5	122.8
Rou15	14.95%	9	**13.44%**	13	15.81%	7	47.5	134.1
Rou20	16.97%	25	**16.17%**	27	17.75%	16	53.8	152.2
Scr12	**7.44%**	5	7.92%	6	8.79%	3	2.5	0
Scr15	**10.18%**	8	10.59%	10	11.72%	5	3	0
Scr20	**16.16%**	16	16.52%	19	17.29%	9	3.5	0
Tai12b	**9.95%**	7	27.73%	10	26.86%	5	210.3	0.7
Tai20b	**8.43%**	30	47.22%	37	30.70%	19	420.5	-2.5
Tai25b	**15.69%**	72	24.33%	73	20.93%	34	558.5	-2.5
Tai30b	**12.82%**	120	14.75%	191	15.01%	60	666.1	0.74
Tho30	**12.79%**	73	13.53%	90	13.73%	38	5.5	0

Table 3: Selected bounds for QAPs of small sizes ($n \leq 30$)

	SDRMS-SUM		SDRMS-SVD		SDRMS-ONE			
Prob.	R_{gap}	CPU	R_{gap}	CPU	R_{gap}	CPU	α	β
Kra32	**18.49%**	97	18.59%	212	19.27%	61	207.5	0
Sko42	**7.75%**	309	8.04%	521	8.29%	119	5.5	0
Sko49	**7.03%**	704	7.44%	954	7.69%	251	6	0
Sko56	**7.05%**	1447	7.25%	2114	7.50%	483	6.5	0
Sko64	**6.40%**	2861	6.72%	4449	6.82%	903	7	0
Ste36a	**19.19%**	194	19.57%	242	19.60%	85	5.5	0
Ste36b	**18.56%**	193	24.20%	266	58.62%	132	49.9	36.1
Ste36c	**14.64%**	342	18.08%	349	15.32%	157	5390.6	-380.6
Tai35b	**14.52%**	307	21.68%	308	17.08%	119	584.2	-2.1
Tai40b	**11.43%**	537	14.57%	767	14.38%	213	797.8	-3.6
Tai50b	**13.79%**	1421	16.86%	2348	15.61%	598	969.2	-5.3
Tai60b	**10.82%**	3390	18.65%	6214	15.21%	1022	1090.5	0.5
Tai64c	61.31%	2201	**3.25%**	3843	61.3%	592	0.5	11.0
Tho40	**12.91%**	280	13.44%	322	13.65%	119	5.5	0
Wil50	**4.01%**	721	4.16%	1047	4.38%	275	6.5	0

Table 4: Selected bounds for QAPs of median sizes ($30 < n \leq 70$)

	SDRMS-SUM		SDRMS-SVD		SDRMS-ONE			
Prob.	R_{gap}	CPU	R_{gap}	CPU	R_{gap}	CPU	α	β
Sko72	6.04%	561	6.29%	828	6.60%	330	7.5	0
Sko81	5.90%	787	6.17%	982	6.33%	477	8	0
Sko90	5.63%	1113	5.85%	1501	6.08%	512	8.5	0
Sko100a	5.37%	1582	5.65%	1921	5.85%	806	9	0
Sko100b	5.44%	1467	5.79%	1932	5.83%	745	9	0
Sko100c	5.40%	1530	5.75%	1962	5.91%	734	9	0
Sko100d	5.54%	1652	5.85%	2041	5.95%	778	9	0
Sko100e	5.54%	1490	5.83%	1999	6.05%	838	9	0
Sko100f	5.60%	1434	5.98%	2083	5.86%	818	9	0
Tai80b	12.28%	762	17.48%	1272	14.79%	521	853.7	-0.3
Tai100b	10.78%	1885	19.75%	2210	14.32%	1375	968.3	0.3
Tai150b	11.45%	3292	12.10%	7005	14.32%	2935	106.9	5.7
Tho150	6.65%	4775	7.02%	5749	7.13%	2112	11.5	0
Wil100	3.15%	1438	3.26%	1820	3.41%	867	9	0

Table 5: Selected bounds for QAPs of large sizes ($n > 70$)

	OPT/Feas	SDRMS-SUM Bound	R_{gap}
Sko90	115534	109030	5.63%
Sko100a	152002	143846	5.37%
Sko100b	153890	145522	5.44%
Sko100c	147862	139881	5.54%
Sko100d	149576	141289	5.54%
Sko100e	149150	140893	5.54%
Sko100f	149036	140691	5.60%
Tai35b	283315445	242172800	14.52%
Tai40b	637250948	564428353	11.43%
Tai50b	458821517	395543467	13.79%
Tai60b	608215054	542376603	10.82%
Tai80b	818415043	717907288	12.28%
Tai100b	1185996137	1058131796	10.78%
Tai150b	498896643	441786736	11.45%
Wil100	273038	264442	3.15%

Table 6: New best known bounds for QAPLIB instances

schemes. Even for the three selected splitting schemes, we could not find any dominative relationship among them. Further study is needed to address such an issue.

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